ECOTOX

ECOTOXicology Database System

ECOTOX Chemical Verification and Entry Procedure

Prepared for:

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Chemical Module - Table of Contents

ACCESS

The Chemical module can be accessed through the ECOTOX Unify dashboard upon login. To enter, select the Chemical module icon. All users have read access to search for chemicals, view chemicals and view chemical information. To enter, edit or verify records, you must have that role assigned by a data base administrator.

SEARCH

The search function allows users to search by the following data types:

- Chemical/Alternate Name (Starts with, Contains, Exact, and Match Case)
- Molecular Formula (Starts with, Contains, Exact, and Match Case)
- Chemical Abstract Service (CAS) Registry Number
- Dates (Created, Modified and Archived)
- Chemical Group
- Chemical Status (Incomplete, Unverified, Verified, and Deleted/Alternate CAS Number)
- Record Status (Created, Modified, and Archived)
- Record Type (Active, Inactive and Archived)
- Report Type (Excel or HTML)
- Priority References Only (returns only unverified chemical names from priority references)

NAVIGATION

In addition to the search functions, the following icons are used in the navigation of the chemical module:

Icon	Description	Function
	Magnifying glass	Print View
	Binoculars	Search
	Pencil	Edit View
	Page with 'X'	Delete
	Plus Sign/Add Button	Add
	Right Arrow	Hover over to display complete text
	Page with Check	Verify

Icon	Description	Function
	Circle with Slash	Reject Chemical Verification
	Printer	Print Command
	Excel Sheet	Download to Excel
	Circle Arrow	Return to search screen
	Circle 'i'	Hover over to display modified information

OVERVIEW

The purpose of the chemical files is to integrate a verified chemical, structure and physical properties list into the MED ECOTOXicology Systems software. Chemicals identified through literature review for the ECOTOX databases are verified by ECOTOX staff members and the acquired information is stored in the Chemical Module of Unify, the chemical verification and information data file.

The following documentation details the verification procedures and describes the format of the chemical information data files.

The Chemical Abstracts Services Registry Number (CAS #) is the core of the verification procedure. Each chemical in the database must have a CAS # assigned prior to data entry. The chemical files are linked between ECOTOX software modules by the CAS registry number. The CAS # also provides a link to the Collective Index (CI) name which is stored in the Chemical Module as the Preferred Name (PN). The Chemical Module strives to use the 9th Collective Index Name as its preferred name.

The Chemical Module is accessible to ECOTOX users to assist in linking CAS #s and chemical names to toxicity data. Chemical or physical property data are also stored in the Chemical Module file.

The Chemical Module also provides a link to additional US EPA databases and models (refer to the SMILES section of this SOP for further information).

Chemicals Excluded in ECOTOX

Any chemical causing an adverse effect is included into the ECOTOX database.

The following are exclusions for the ECOTOX database. For all of the exclusions listed below, an exception for inclusion into ECOTOX will be made as requested by EPA.

- Effluents
- Chemical mixtures (unless a single concentration and CAS number can be provided)
- Water\Soil chemistry effects, e.g. Hardness or pH (unless caused by a single chemical)
- Biological toxicants (venoms, fungal toxins, Bacillus thuringiensis, and other plant, animal or microbial extracts or toxins not purified)
- Dietary Chemicals (Nutrients) that are not added in excess (authors state either deficient or sufficient diet)
- Oils (crude or synthetic oils, coal, and petroleum based fuel products or distillates, all of which are mixtures. Note that creosote is OK.)
- Air Pollutants
- Proteins and enzymes
- Clay and diatomaceous earth products

Verification Procedure

Each chemical identified during ECOTOX literature skim and/or review is tracked

electronically through the chemical verification process. Each chemical in the data file is verified in one or two chemical name sources (only one source is needed if the source is the Chemical Abstract Services' STN International or the CAS Registry Handbook) and one structure source (Appendices A and B). Chemicals that are not verified through the regular sources are archived. Data associated with unverified chemicals are not entered into ECOTOX.

Minimum Criteria

The minimum criteria for a chemical to be entered into the Chemical Module are a Chemical Abstract Services Registry Number (CAS number) and a preferred name. The Chemical Module Collective Index Name is obtained from either the STN International database or CAS Registry Handbooks available at the MED library, both are indexed by CAS number.

Summary and Flowchart of Verification Procedures

Below are the processes followed to verify chemical information:

1) Search to confirm whether the chemical already exists in the Chemical Module.
2) If the chemical name is not in Chemical Module, identify and verify the CAS number, preferred name, synonym(s), chemical and physical property data and structure information.
   a. Conduct a STN Search for unverified chemicals
      i. Located and not trade name, proceed to step 3
      ii. Located and trade name
         1. Author provides additional information (e.g. another name or molecular formula that confirms the STN match, proceed to step 3.
         1. 2. If the trade name in STN does not match the information that the paper provides, it should be further researched to confirm which source appears to be correct. If STN appears to be incorrect, they should be contacted via email (help@cas.org). The email should contain in detail the discrepancy and chemical product labels and/or MSDS links should be provided along with the paper citation information. STN has fixed discrepancies reported in the past. For example, DCT was reported in the paper as diazinon + captan + thiophanate-methyl. STN listed DCT under diazinon-captan-thiophanate-ethyl. Upon further research, the paper appeared to be correct. STN was notified and updated their records accordingly. If STN's response does not fix the discrepancy then each chemical should be handled on a case by case basis on how to verify/skim/code. If the author does NOT provide additional information to confirm STN match, proceed to step b.
   b. If chemical information is not found on STN, additional verification sources are checked (the most common and reliable sources are listed below, all additional sources are listed in Appendix A).
   c. Archive Unverified Chemicals if all sources are investigated and no

verification source contains information.
3) Perform Data Entry of Chemical into the Unify Chemical Module.
4) Complete Quality Assurance of Verified Chemical Information.

Search Unify Chemical Module for Author reported name. Double check author spelling.

Name not in Chemical module. Search STN International database

Name in Chemical module. Forward CAS number to reviewer via dashboard.

Chemical in STN International as valid name.

Chemical in STN International as Trade Name and author provides additional information

Chemical not in STN International or in STN but only Trade Name provided by author

Search other verification sources listed in Chemical Verification file.

Enter information into Chemical module and submit for verification QA.

Chemical name verified in additional source(s). See detailed procedure for number of sources required.

Chemical name not verified in additional sources.

Submitted Chemical record QAed and released as verified.

Chemical record archived as unverified.

Archive determination forwarded to reviewer via dashboard.

Figure 1. Chemical Verification Flowchart

Verification Sources

Verification sources are used to verify chemical name, synonym CAS number, and structural or physical property information. STN International is the preferred source for chemical verification. The refe rence number, database location and complete citation of verification publications are listed in Appendices A and B. Appendix C documents additional rules to aid the verification process. The following sources are most commonly used and reliable for verification of chemical name spelling and CAS numbers:

- STN International (ECOREF#1329)
- ChemBioF inder (www.chembiofinder.com) (ECOREF#58458)
- Sigma-Aldrich on-line catalog (www.sigma-aldrich.com) (ECOREF#58784)
- RTECS (Registry of Toxic Effects of chemical substance, 1983-84 edition, 2 volumes) (ECOREF#13337)
- TSCA (Toxic Substances Control Act Chemical Substance Inventory, 1985 edition, 5 volumes) (ECOREF#13318)
- Dictionary of Chemical Names and Synonyms (1992) (ECOREF#4062)
- The Pesticide Manual 10th edition (1994) (ECOREF#1012)
- The Compendium of Pesticide Common Names website (http://www.alanwood.net/pesticides/(ECOREF#89844)

VERIFICATION PROCEDURES (SPECIFIC STEPS)

Each chemical identified during ECOTOX skim is tracked through the chemical verification process electronically. All chemicals are searched via STN International database (see Appendix D). Each chemical in the data file is verified in one or two chemical name sources (only one source is needed if the source is the Chemical Abstract Services or STN International reference) and one structure source (Appendices A and B). Chemicals that are not verified through the regular sources will be archived. Data associated with unverified chemicals are not entered into ECOTOX.

If the chemical name from the paper is a trade name, and no other chemical information is given by the author, in addition to STN, the chemical must be verified in an additional source. If the author provides the chemical company that produces the product, CSC will attempt to access the company's web site for additional information about the chemical.

Chemical Degradates, EPA IDs and Use should be researched for prior to starting a New Chemical entry in Unify.

Chemicals submitted through the skimming process

1. Verification staff will retrieve the Incomplete (skim) chemicals to be verified from their dashboard. Prioritized chemicals can be searched by selecting the "Priority References Only" check box in the Search Chemicals screen of the Chemical module or via a custom query searching for upcoming priority chemicals.
2. Select the chemical to be verified by selecting the edit icon.
3. Verify chemical name via the Chemical verification flow chart (Figure 1).
4. If chemical cannot be the verified with a CAS number, note "NO 'sources' 'month/year' in the Notes Tab and select the Save Note button. Select the Archive button from the Status section and skip remaining steps listed below. Review the chemical in the paper for additional information. If the author reports the active ingredient associated with the chemical name, instruct the reviewer to code as the active ingredient and note the chemical name in the Chemical Comments data field.
5. If the chemical CAS number is found, add the CAS Number and verification source to the Chemical Name record and click Submit Changes.
   a. If the CAS number exists in the system, it will ask if this name should become an Alternate Name for the existing CAS Number. Follow prompts to update the record.
   b. If the CAS Number does not exist in the system, it will ask if you want to be redirected to the Add Chemical screen. Select ok. Add the CAS number to the text box and select submit. Continue to Step 6 and follow additional instructions in Step 10.
6. Update chemical details (e.g., Collective Index name, Molecular Formula, etc.) into the appropriate data fields. Click the Submit Changes button otherwise this information will not be saved.7. Update chemical Degradates, EPA IDs, Uses, Notes and AR/DR numbers (AR/DR instructions see Appendix G) for the

chemical.

8. Create a text file containing the information from STN and attach to the record.
9. Select Submit for Verification from the Status section.
10. If the original chemical name's CAS Number did not exist in the system, retrieve the original Incomplete (skim) chemical name to be verified from the dashboard in order to link it to the newly created CAS number record. Enter the CAS number and reference. The system will ask if this name should become an Alternate Name for the existing CAS Number. Follow prompts to update the record.
11. Verify and release Chemical to Unify (see VERIFICATION QUALITY ASSURANCE).

Chemicals submitted outside skimming process

1. If a chemical name is received from an outside source (e.g. upcoming priority chemical) and is not found in the Unify Chemical system complete verification of the chemical name via the Chemical verification flow chart (Figure 1).
2. If a chemical cannot be verified with a CAS number, select Add New Chemical and select Insert Blank CAS Number. Enter the chemical name and note "NO 'sources' 'month/year' " in the Notes Tab and select the Save Note button. If the chemical is an EPA Pesticide Fate Database degradate, designation should also be noted with a comment that 'no papers have been found to be associated with this chemical' in the Notes Tab. Select the Submit for Verification button from the Status section and skip remaining steps listed below.
3. If chemical CAS number is found, search the chemical CAS number.
   a. If the chemical CAS number is in the Unify system, select the chemical to be verified by selecting the edit icon.
   b. If the chemical CAS number is not in the Unify system, select Add Chemical from the left hand chemical tab. Add the CAS number to the text box and select submit.
4. Update chemical details (e.g., Collective Index name, Molecular Formula, etc.) into the appropriate data fields, if needed. If any changes have been made, click the Submit Changes button otherwise this information will not be saved.
5. Select the plus sign in the Alternate Names section, add chemical name and reference.
6. Update chemical Degradates, EPA IDs, Uses, Notes and AR/DR numbers (AR/DR instructions see Appendix G) for the chemical.
7. Create a text file containing the information from STN and attach to the record.
8. Select Submit for Verification from the Status section.
9. Verify and release Chemical to Unify (see VERIFICATION QUALITY ASSURANCE).

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DATA FIELDS AND ENTRY INTO THE UNIFY CHEMICAL MODULE

Data Fields

The chemical screen is divided into four sections; Status, Details, Alternate Names and Chemical Information. Data fields in each section and their entry/navigation are detailed below.

Status Section

- Record History: The Unify system electronically notes the most recent activity for each record.

- Status: The Unify System tracks the Status, (e.g. Incomplete, Unverified, Verified, or DR/AR) of each chemical electronically.

- Record Type: The Unify system electronically catalogs the chemicals as Active, Inactive, or Archived.

- Record Status: The Unify System tracks the Record Status, (i.e. New, Modified or Deleted) of each chemical electronically.

- Chemical Name - Verified/User: The Unify system provides the verification status of Chemical Name verification and the person who completed the verification.

- Properties - Verified/User: Provides the verification status of Chemical Properties verification and the person who completed the verification.

- SMILES - Verified/User: Provides the verification status of SMILES information verification and the person who completed the verification.

Buttons/Icons

Icon	Description	Function
DR/AR	DR/AR	Selecting this button will cause the chemical to be moved to the Deleted or Alternate Registry number status. If the chemical is changed to this status, the CAS Number needs to be added to the Historical CAS tab of the Chemical Information (tabbed section).
Archive	Archive	Archives the chemical for future verification (See archived chemical processing for further information)
Archive – Under AI	Archive – Under AI	Archives the chemical for future verification (See archived chemical processing for further information) but the chemical will be coded under the Active Ingredient (AI) if reported by the author.

Icon	Description	Function
Delete	Delete	Deletes the existing chemical from the Chemical Module.
Activate Chemical	Activate Chemical	This selection will reactivate a record that had been changed to a DR/AR, Deleted or Archived status.
Submit For Verification	Submit For Verification	This selection is made once all of the data fields and been entered for a new chemical only. The chemicals set to this status will appear on the Verifier's dashboard for verification processing. Any chemical that has been previously entered and verified and edited will automatically display on the Verifier's dashboard for verification.
	Circle 'i'	This icon reveals the data fields that have been modified for verification

Details Section

- CAS Number: Chemical Abstract Services Registry Number - unique identifier for each chemical. Enter the CAS Registry Number.

- Solvent: Selection box that denote that the chemical is used as a solvent. This selection should be made if the chemical was used as a solvent/carrier for any paper.

- Chemical Structure: 2D depiction of the chemical structure (if SMILES provided)

- CI Name/References: Selection box that denotes the name is a Collective Index name and its associated references. Both references should contain entries unless the verification source is STN International or Chemical Abstract Service Registry Handbooks.

- Chemical Name: The Collective Index name must be obtained from at least one verification source; the CAS Registry Handbook or STN International, the Collective Index name. All associated Alternate Names, CAS Number, Molecular Formula, Structural and Physical property data and the SMILES String are linked electronically to this name in the ECOTOX databases.

- The Marked for Delete selection box is for Data Maintenance staff in the event that the Chemical Name is found to be incorrect. If the boxed is checked, the Chemical Name cannot be selected for skimming/reviewing.

- Tested SMILES (Unique SMILES - Display only)/Reference: SMILES strings are written for chemicals entered into the Ecotoxicology databases. A SMILES string is a linear representation of a chemical structure that is computer recognizable and can be used to search the chemical in the Ecotoxicology databases. The SMILES String of the compound and it associated reference and page number of the structure image are entered. If a SMILES string cannot

be written, a designator is determined (See Appendix F).

SMILES strings are written by the designated personnel using guidelines from one of the following sources:

- Russom, Christine L. 1990. Appendix B. SMILES Tutorial. IN: ASTER Users Manual, ERL-Duluth. (See Appendix E: SMILES TUTORIAL)

- Anderson, E., G.D. Veith, and D. Weininger. 1987. SMILES: A line notation and computerized interpreter for chemical structures. Report No. EPA/600/M-87/021. U.S. Environmental Protection Agency, Environmental Research Laboratory-Duluth, Duluth, MN 55804

- Hunter, R.S., F.D. Culver, and A.Fitzgerald. 1987. SMILES User Manual. A Simplified Molecular Input Line Entry System. Includes extended SMILES for defining fragments. Review Draft, Internal Report, Montana State University, Institute for Biological and Chemical Process Control (IPA), Bozeman, M.T.

- Modeled SMILES (Unique SMILES - Display only)/Reference: The SMILES String used in the modeling software. Usually the same as the Tested SMILES string, but may be entered by removing a disconnected salt or only the active part of the compound.

- Molecular Formula/Reference: Molecular formula identifies each constituent element by its chemical symbol and indicates the number of atoms of each element found in each discrete molecule of that compound, with the associated reference. If the molecular formula cannot be verified the Unspecified check box is selected to denote the formula is unspecified.

Buttons/Icons

Icons	Description	Function
	Binocular	Activates the Reference search page to locate the EcoRef Number of the verification source. You can also type in the EcoRef Number if known. When the reference is retrieved, select the Plus Sign to select the reference and close the search window.
Clear Changes	**Clear Changes**	Removes all changes made during current session.
Submit Changes button	**Submit Changes button**	Saves edits made to the Chemical Details section.

Alternate Names Section

- Alternate Chemical Names are obtained from the publication, and entered into

the chemical work flow during the skimming process (see ECOTOX Literature Searches, Citation Identification and Skimming SOP). During skimming, a new chemical name will be entered and electronically attached to the reference. The Alternate Name must be verified in two sources unless one is STN International. Alternate Names include synonyms, product IDs, etc. To View/Edit a chemical name, highlight and click the name. To add names select the Plus Sign icon. The Alternate Name view/edit screen contains a <u>Marked for Delete selection box. This is available for Data Maintenance staff in the event that the Alternate Name is found to be incorrect. If the boxed is checked, the Alternate Name cannot be selected for skimming/reviewing.</u>

Buttons/Icons

Icon	Description	Function
	Plus Sign	Opens the Alternate name entry screen
	Page with X	Deletes the selected Alternate name
	Binocular	Activates the Reference search page to locate the EcoRef Number of the verification source. Alternately, type in the EcoRef Number if known. Search for the reference, select the Plus Sign and the reference number will be transferred.
Cancel	**Cancel**	Exits the Alternate Name entry screen without committing changes.
Add	**Add**	Commits the edits to the Alternate name and references.

Chemical Information Section (Tabbed)

PROPERTIES TAB

The format of the entries for most of the following data fields are in the format of mathematical Operator, numeric Value, Units and the associated verification Reference. Enter these data fields as needed. Include verification information into a document that can be attached the chemical for QA. See Appendix A for verification sources of properties.

- MolecularWeight: Calculated from the Molecular formula in the Chemical Details section.

  The Molecular Weight data field may be over written in some instances. To over write the value, check the Edit box. This opens the data field to editing.

- TMOA (Toxic Mode of Action): A common set of physiological and behavioral

signs that characterize a type of adverse biological response. Seven major modes of toxic action include non-polar narcosis, polar narcosis, uncouplers of oxidative phosphorylation, acetylcholinesterase (AChE) inhibitors, irritants, a general group of central nervous system seizure agents, and respiratory blockers (Rand, 1995).

This value is generally calculated from the modeling system (ASTER). In some instances, the TMOA is overridden by selecting and storing the TMOA on the Properties Tabs. This override is directed by EPA.

- Melting Point: Melting point is the temperature at which crystals are in equilibrium with the liquid phase at atmospheric pressure. The terms melting point and freezing point are used interchangeably, depending on whether the substance is being heated or cooled (Hawley, 1981.)

- Boiling Point: Boiling point is the temperature at which the vapor pressure of a liquid is equal to the pressure of the atmosphere (Rechsteiner, 1982a). The model used for estimating the boiling point of chemicals is the Meissner method (Rechsteiner 1982a).

- Vapor Pressure : Vapor pressure is the pressure in mm of mercury at which a solid is in equilibrium with its own vapor.

- Vapor Pressure Temperature: The temperature at which the vapor pressure is reported.

- Molar Refraction (Henry's Constant): Molar Refraction (Henry's Constant) is the ratio of chemical concentration in air to concentration in water, when those two phases are in contact and are at equilibrium (Thomas 1982.)

- Log P: Log P (the Logarithm of the Octanol-Water partition coefficient) is the equilibrium concentration of solute in a non-polar solvent (octanol) divided by the concentration of the same species in a polar solvent (water; Leo and Weininger, 1984).

- Water Solubility: Solubility reflects the maximum amount of chemical that will dissolve in pure water at a given temperature (Lyman, 1982).

- pKa Value: pKa is an expression of the strength of an organic acid or base (Perrin et al., 1981). pKa is estimated using an algorithm by Hunter (1988) based on Perrin et al. (1981).

- LogKoc (Adsorption Coefficient): The Adsorption Coefficient (Log Koc) is the ratio of soluble fugacity coefficients in the aqueous and organic matter phase (Lyman, 1982b.)

Buttons/Icons

Icon	Description	Function
	Binocular	Activates the Reference search page to locate the EcoRef Number of the verification source. Alternately, type in the EcoRef Number if known. Search for the

Icon	Description	Function
		reference, select the Plus Sign and the reference number will be transferred.
Clear Changes	Clear Changes	Removes all changes made during current session.
Submit This Tab	Submit This Tab	Commits all edits made to the Properties tab.

DEGRADATES

Chemical degradates for the chemical and it associated reference. The primary source of degradate information is the EPA Pesticide Fate Database (http://cfpub.epa.gov/pfate/E_AChemicals.cfm).

To add a degradate, select the Plus Sign icon, perform the chemical search for the degradate. Select the degradate from the retrieved chemicals by adding a reference to the degradate's search result and select the Plus Sign to add and close the Chemical Search screen. If the chemical is not retrieved, the degradate must be verified and added to the Chemical Module prior to selecting the degradate for the Degradate tab.

Buttons/Icons

Icon	Description	Function
	Plus Sign	Opens the Chemical Search screen
	Page with X	Deletes the selected Degradate
	Binocular	Activates the Reference search page to locate the EcoRef Number of the verification source. Alternately, type in the EcoRef Number if known. Search for the reference, select the Plus Sign and the reference number will be transferred.

CHEMICAL GROUPS

Chemical group can be defined by a Chemical of Concern (COC) code, specific project, e.g. EFED, or by chemical element, e.g. As – Arsenic.

To add a Chemical group, either select the chemical from the Chemical Groups dropdown menu or search for the chemical group by selecting the binocular icon. If the Group has been selected from the dropdown menu, select the Add button to commit the group. If the group was retrieved from the search function, select the Plus Sign icon to add the group and close the search window.

If the Chemical Group code needs to be added, the Binocular icon will link to the code

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validation file. The code must be added before the group can be selected.

Buttons/Icons

Icon	Description	Function
	Page with X	Deletes the selected Chemical Group
Add	**Add**	Commits the selection made from the Chemical Group selection box.
	Binocular	Activates the Chemical Groups Validation search page to add or locate the Chemical Group Code(s). Select the Plus Sign to select the code(s) and close the search window.
	Plus Sign	Selects and commits the retrieved Chemical Group Code(s)

Chemical groups can also be added using **Assign Chemicals to Groups** located on the Chemical home page or the navigation links expanded under **Chemicals** within the Unify dashboard. By using this section, multiple chemicals can be added to a chemical group, rather than one chemical at a time.

To add multiple chemicals to a group:

1. Select the group to be added to from the Select Group box (first selection box). When selected, chemicals belonging to the group will appear in the Chemicals in Selected Group box.

2. Search for additional chemicals by selecting the Binoculars icon and perform the search needed to populate the group. Multiple chemicals can be searched as long as they are comma separated.

3. Select retrieved chemicals by clicking the box in the first cell of each record that belongs to the group. If all are to be added, select "All" at the top of the list. "None" will clear all selections.

4. Select **Add Selected Chemicals to Group** to commit the chemicals to the group. The search window will stay open to search for additional chemicals until closed by the user.

Buttons/Icons

Icon	Description	Function
	Page with X	Deletes the selected Chemical from the Group from the Chemicals in Selected Group selection box.

Icon	Description	Function
Binocular	Binocular	Activates the Chemical search page to locate chemicals to add to groups.
Add Selected Chemicals to Group	Add Selected Chemicals to Group	Commits the selections from the search retrieval to the Group
All	All	Selects all records retrieved in the chemical search.
None	None	Clears any previous selections in the records retrieved from the chemical search.

EPA IDs

U.S. EPA PC (Pesticide Chemical) Code is a unique chemical code number assigned to a particular pesticide active ingredient or mixture of active ingredients. The primary sources for EPA IDs are the California Department of Pesticide Regulation website (http://www.cdpr.ca.gov/docs/monster/monster.htm) and the Dictionary of Chemical Names and Synonyms CDROM (1998).

Buttons/Icons

Icon	Description	Function
Page with X	Page with X	Deletes the selected EPA ID
Add	Add	Commits the entries in EPA ID and Verify ref fields.
Binocular	Binocular	Activates the Reference search page to locate the EcoRef Number of the verification source. You can also type in the EcoRef Number if known.
Plus Sign	Plus Sign	Selects the retrieved EcoRef reference and inserts the number into the Verify Ref field.

CONC TYPES

Codes that denote that the concentration is based on the active ingredient or formulation for organic compounds, or as the total, un-ionized or dissolved concentration, for metal, ionic or organo-metallic compounds as a validation source for the Concentration Type data field in the Toxicity Module.

Metals are defined by the concentration types, total (T), dissolved (D), and labile/free (L); while ammonia or hydrogen sulfide compounds may have total concentrations (T) and/or un-ionized (U) concentrations. Organometals are compounds that contain covalent bonds between carbon atoms and metal atoms and are coded as total (T) concentrations.

Based on the Molecular Formula (or chemical notes for chemicals that have unspecified Molecular Formulas) the Verifier will select the Concentration Type Codes allowable for the chemical from the dropdown list. All approved Concentration Type Codes are shown in the dropdown. If the Molecular Formula is unspecified and there are no notes as to the composition of the compound, the Concentration Types of A and F will be selected by default. In future versions, it is proposed that the system will assign the Concentration Types based on the Molecular Formula and the Verifier will modify them based on the Notes or confirm the Chemical Modules assessment.

EPA must prior approve new Concentration Type codes. Approved codes can be added by selecting the Binocular icon which opens the code validation file in a new window. The code must be added before the Concentration Type can be selected from the dropdown box.

Buttons/Icons

Icon	Description	Function
	Page with X	Deletes the selected Concentration Type
	Add	Commits the selection made from the Concentration Type selection box.
	Binocular	Activates the Concentration Type Validation search page to add an approved Concentration Type Code. Select the Plus Sign to select the Concentration Type and close the search window.
	Plus Sign	Adds new Concentration Type from Concentration Type Validation page.

ION CODES

All constituent elements by chemical symbol are added to Ion Codes as a validation source for the ion data field in the Toxicity Module.

Based on the Molecular Formula (or chemical notes for chemicals that have unspecified Molecular Formulas) the verifier will select the Ion Codes allowable for the chemical from the dropdown list. All approved Ion Codes will show in the dropdown. If the Molecular Formula is unspecified and there are no notes as to the composition of the compound, no Ion codes will be noted. In future versions, it is proposed that the system will assign the Ion Codes based on the Molecular Formula and the verifier will modify them based on the Notes or confirm the Chemical Modules assessment.

If an Ion code needs to be added, the Binocular icon will link to the code validation file. The code must be added before the Ion Code dropdown can be selected.

Buttons/Icons

Icon	Description	Function
	Page with X	Deletes the selected Ion Code
Add	Add	Commits the selection made from the Ion Code dropdown box.
	Binocular	Activates the Ion Code Validation search page to enter a new Ion Code or select multiple codes. Select the Plus Sign to select each Ion Code and close the search window.
	Plus Sign	Adds new or retrieved Ion Code from Ion Code Validation page.

REFERENCES

This tab will display the Reference Number, Title, Author, Source, Database (AQUIRE and/or TERRETOX) and Publication Year for the verification source for each entry, e.g. Chemical Name, SMILES String, Boiling Point, etc.

Buttons/Icons

Icon	Description	Function
	Page with Arrow	The data in this field has been truncated for display. Mouse over the icon to view the entire value.

CHEMICAL USE

The most common uses for a pesticide active ingredient, e.g. herbicide, are entered. The primary source of Use information is the PAN (http://www.pesticideinfo.org/Search_Chemicals.jsp#ChemSearch).

To add a Use either select the use from the Uses dropdown box or search the Uses Validation codes and select the code by clicking the Plus Sign to add and close the Uses screen. If the Use is not retrieved, the Use must be verified and added to the Uses Validation file prior to selecting the degradate for the Degradate tab.

If the Use code needs to be added, the Binocular icon will link to the code validation. The code must be added to the validation file before the Uses can be selected.

Buttons/Icons

Icon	Description	Function
	Page with X	Deletes the selected Use

Icon	Description	Function
Binocular	Binocular	Activates both the Uses Validation search page and the Reference search page. Locate the Uses code and select the code by clicking the Plus Sign to transfer to the Current Uses field. Locate the EcoRef Number of the verification source. You can also type in the EcoRef Number if known. Search for the reference and select the Plus Sign to transfer the reference number to the field.
Add	Add	Commits the selection made from the Uses selection box.
Plus Sign	Plus Sign	Selects the retrieved Uses Code or Reference.

NOTES

Notes about the chemical entry, e.g. if the same name is used for more than one CAS Number, sources that were checked for verification, or chemical make-up if the molecular formula is contains a 'n' or 'x' (unspecified ratio of ions), etc. are stored.

Enter the text to be saved to the record in the text box.

Buttons/Icons

Icon	Description	Function
Save Note	Save Note	Commits the notes that have been added to the chemical.

ATTACHMENTS

An area of the chemical record to upload the verification sources for each chemical entry, this may include a file of the website used for verification.

To add attachments select the Plus Sign to open the file browser. Search for the files to add. Once located, select the Save Attachment button to commit. A Note area is also available to describe the different attachments, e.g. Boiling Point.

Buttons/Icons

Icon	Description	Function
Plus Sign	Plus Sign	Opens the Browse File window.
Browse	Browse	Opens file explorer window to search for files.
Save Attachment	Save Attachment	Uploads and saves the attachment to the notes entry.
View	View	Opens attachment in Read Only mode.
Page with X	Page with X	Deletes the selected attachment

HISTORICAL CAS

- CAS Number/Reference : The Chemical/CAS Number that has been deleted or is an alternate name and its associated reference. The CAS Number can be appended if existing records are stored or Overwritten as needed by selecting one of the two radio buttons.

- Reason: Notes if the Name/CAS number is a Deleted or Alternate number. Select the Reason from the Reason dropdown field.

Buttons/Icons

Icon	Description	Function
Page with X	Page with X	Deletes the selected Historical CAS number selected.
Binocular	Binocular	Activates the Reference search page to locate the EcoRef Number of the verification source. You can also type in the EcoRef Number if known. Search for the reference and select the Plus Sign to transfer the reference number.
Add	Add	Commits the edit made from Historical CAS tab.

EFED

This tab allows the selection of the name that should be used in the EFED reports.

ARCHIVAL OF UNVERIFIED CHEMICALS

If the STN search and other sources listed in Appendix A do not provide a CAS number for the chemical name or structure, several additional steps should be taken:

1. Recheck the original paper for accurate spelling and any additional chemical information (active ingredients, formula, synonyms, etc.). Search the bibliography for chemical references. If the author reports the active ingredient associated with the unverified chemical name, instruct the reviewer to code as the active ingredient and note the chemical name in the Chemical Comments data field.

2. Conduct an STN chemical search on the new information found.

3. Check additional verification sources for the new information.

4. If, after an exhaustive search, a CAS number is not found, set the chemical status to Archived. An exhaustive search includes checking printed sources and online sources for the chemical name as well as for probable chemical names (e.g., spelling errors in the chemical name), or contacting the author and/or the chemical manufacturer for more information.

   a. If the chemical is the only test chemical in the paper, reskim the paper and add the KEYWORD "CAS# UNAVAILABLE and process. (See Reference Module SOP for specific procedures. Process the entire paper as any other deleted reference.)

   b. If there are other test chemicals, in addition to the Archived chemical(s) in the publication, the verified chemicals will be entered into the system with the following modifications:

      i. The archived chemical name(s) will be put into the Other Effects field individually if n<=5 chemicals. If more than five chemicals are unverified, ">n= other chemicals tested" will be put into the Other Effects field. This statement may be modified to include the chemical type if noted in the paper, e.g., "6 surfactants and 4 emulsifiers tested." This information will also be noted on the front of the publication.

      ii. The total test status will be evaluated and modified if necessary.

   c. If the chemical name appears to be incorrect or a structurally impossible name, contact the author. If there is no response to the chemical inquiry, forward the chemical name and paper to the EPA Database Manager for final approval for archiving. Archiving will follow the same procedure as outlined above, starting at step # 4.

5. Every two years, the Archived chemicals will be re-searched on STN to ensure that the Chemical Abstract Services has not assigned a CAS number to an existing name, or recognized a name as a synonym.

VERIFICATION QUALITY ASSURANCE

Chemicals to be verified upon completion of modifications can be access either through the Quality Assurance Verifier's dashboard or from the link Verify Chemicals on the left column or from the Chemical home page.

From the dashboard:

1. Select the chemical to verify. This will bring the Quality Assurance Verifier to the individual chemical record.

2. QA Verifier will look at the status area to note which areas have been modified; Chemical Name, Properties or SMILES. Specific fields edited are list and can be viewed by hovering the cursor over the "Circle I" icon.

3. QA Verifier will review the notes and attachments to verify the entries/edits made. Each field and tab is looked at and compared to available documentation with special attention to the spelling of chemical names

4. QA Verifier will select the Paper with Check icon to verify the record or reject the edit by selecting the Circle with Line icon for each section as needed. If rejected, a Prompt box will pop-up and the reason for rejection should be added. The chemical and reason for rejection will reappear on the Verification Staff's dashboard for further review and modifications.

Electronic quality assurances have been built into the Chemical module. The QA features eliminate/stop duplicate CAS numbers from being added to the Chemical module or chemical groups. They also ensure that records are in DR/AR status prior to allowing Verification Staff the ability to attach the deleted/alternate CAS Number to the Preferred CAS Number.

APPENDIX A: SOURCES OF VERIFICATION FOR CHEMICAL NAMES AND STRUCTURES

CHEMICAL SOURCE	SOURCE NUMBER	CONTENTS	DOCUMENT LOCATION
Agrochemicals Handbook (Royal Society of Chemistry) 1983	5716	Pesticide information, CAS numbers and synonyms	ECOTOX
Aldrich Catalog Handbook 94-95	4292	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Aldrich Catalog Handbook 92-93	4294	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Aldrich Catalog Handbook 83-84	59183	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Aldrich Catalog Handbook 92-93	1009	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Alfa (1990-1991)	7677	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Analysis of PCB Congeners	9451	PCB Congeners CAS only	ECOTOX
ChemBioFinder Web site (www.chembiofinder.com)	58458	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	Online

CHEMICAL SOURCE	SOURCE NUMBER	CONTENTS	DOCUMENT LOCATION
Chemcyclopedia-91	1333	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Chemical Information Service (CIS) 1992	3915	Organic and inorganic Compounds by chemical name, has CAS index and structure data	Online system
Chemical Abstracts Services Registry Handbook (numerous volumes)-1965	5713	CAS Numbers and Chemical Module Preferred Collective Index Name	MED Library
CRC Handbook of Data on Organic Compounds	9825	Organic Compounds by chemical name and synonyms, has CAS index, Structure and Physical Property data	UMD Lib.
Crop Protection Chemicals Reference	1336	Pesticide information, CAS numbers and synonyms	ILL
Dictionary of Chemical Names and Synonyms	4062	Wide assortment of chemical compounds by chemical name and synonym, has CAS index and some structure data	ECOTOX
Dictionary of Organic Chemicals (CDROM)	59184	Organic Compounds by chemical name and synonyms, has CAS index, Structure and Physical Property data	CDROM
Dictionary of Inorganic Chemicals (CDROM)	4295	Inorganic Compounds by chemical name and synonyms, has CAS index, Structure and Physical Property data	CDROM
Dictionary of Organic Chemical -1982	59182	Organic Compounds by chemical name and synonyms, has CAS index, Structure and Physical Property data	ECOTOX

CHEMICAL SOURCE	SOURCE NUMBER	CONTENTS	DOCUMENT LOCATION
Distributed Structure-Searchable Toxicity (DSSTox) Public Database Network, Version 1.0 (http://www.epa.gov/ncct/dsstox/DSSToxMasterFile.html)	151468	CAS numbers and synonyms, and structure data	Online
Eastman Laboratory Chemicals	8073	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Farm Chemicals Handbook 1994	58206	Pesticide information, CAS numbers and synonyms, some structure data ***Sometimes CAS number presented for a compound is for the main constituent only	MED Lib.
Farm Chemicals Handbook-1992	5327	Pesticide information, CAS numbers and synonyms, some structure data ***Sometimes CAS number presented for a compound is for the main constituent only	ECOTOX
Fluka Chemical Catalog	9826	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
Handbook of Chemical Synonyms and Trade Names	2321	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	UMD Lib.
Handbook of Tables for Organic Compound Identification-1967	1008	Organic and inorganic Compounds by chemical name, has some structure and Physical Property data	MED Library

CHEMICAL SOURCE	SOURCE NUMBER	CONTENTS	DOCUMENT LOCATION
Herbicide Handbook of the Weed Society of America	1327	Pesticide information, CAS numbers and synonyms, some structure data ***Sometimes CAS number presented for a compound is for the main constituent only	MED Library
ICN Biomedicals, Inc.	3047	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
National Pesticide Information Retrieval System (http://ppis.ceris/purdue.edu)	156761	Chemical names, synonyms and PC codes	Online
Merck Index, 11th Edition-1989	5728	Mostly organic compounds by chemical name, has some CAS numbers and some structure and Physical Property data	ECOTOX
MSDS Reference for Crop Protection Chemicals	1337	Pesticide information, CAS numbers and synonyms	ILL
OPPT SMILES Verification Source	150908	Structure Data	ECOTOX
Pesticide Index, 5th Edition-1976	5723	Pesticide information, CAS numbers, synonyms and some structure data	ECOTOX
RTECS fiche (January 1990)	58207	Chemical names, synonyms and CAS numbers	ECOTOX
RTECS (Registry of Toxic Effects of chemical substance, 1983-84 ed., 2 vols)	13337	Chemical names, synonyms and CAS numbers	ECOTOX
Sigma	4293	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX

CHEMICAL SOURCE	SOURCE NUMBER	CONTENTS	DOCUMENT LOCATION
Sigma-Aldrich Library of Rare Chemicals-Structure Index	1001	Structure data only, organized by Aldrich product numbers	ECOTOX
STN International (CAS) 1994	1329	***Most complete source of chemical name, synonym and structure information, no physical properties	Online
TCI America	9679	Organic and inorganic Compounds by chemical name, has CAS index and some structure and Physical Property data	ECOTOX
The Pesticide Manual 9th edition, 1991	9824	Pesticide Compounds by chemical name, synonym, product code, has CAS index and some structure and Physical Property data	ECOTOX
The Pesticide Manual 10th edition, 1994	1012	Pesticide Compounds by chemical name, synonym, product code, has CAS index and some structure and Physical Property data	ECOTOX
Tracor Jitco (A historical commercial source. No longer used.)	58995	Chemical names, synonyms and CAS numbers	Commercial Source
TSCA (Toxic Substances Control Act Chemical Substance Inventory, 1985 ed., 5 vols)	13318	Chemical names, synonyms and CAS numbers	ECOTOX
World Wide Web (misc. web sources) A copy of the verification page is saved to the Attachments tab of the chemical entry. This includes company MSDS sheets or Chemical Labels.	58886	Chemical names, synonyms and CAS numbers	Online

CHEMICAL SOURCE	SOURCE NUMBER	CONTENTS	DOCUMENT LOCATION
ADDITIONAL SOURCES NOT LISTED IN SOP			
Handbook of Environmental Data on Organic Chemicals – 1977	1002	Organic compounds with chemical name, and has some structure and Physical Property data	MED Library
CRC Handbook of Chemistry and Physics 1982 and 1986	1003	Organic and Inorganic compounds with chemical name, and has some structure and Physical Property data	MED Library
Physical Properties of Compounds (II and III) 1959	1004	Organic and Inorganic compounds with chemical name, and has some structure and Physical Property data	MED Library
The SCS/ARS/CES Pesticide Properties Database for Environmental Decision Making	5739		MED Library
Linear Solvation Energy Relationships. 41. Important Differences Between Aqueous Solubility Relationships for Aliphatic and Aromatic Solutes	1005		
Compendium of Pesticide Common Names (http://www.alanwood.net/pesticides/)	89844	Pesticides listed by common name, CAS #, IUPAC name, and molecular formula. Has some structure information	Online
California Department of Pesticide Regulation (http://www.cdpr.ca.gov/dprdatabase.htm)	89843	Multiple databases containing chemicals, pesticides, companies, products, etc.	Online

CHEMICAL SOURCE	SOURCE NUMBER	CONTENTS	DOCUMENT LOCATION
PAN Pesticide Database (http://www.pesticideinfo.org/IndexContent.html)	89842	Pesticides searchable by name or CAS #. Includes CAS #, Name, synonyms, targets, toxicity data, related chemicals and regulatory information.	Online
US EPA Pesticide Fate Database (http://cfpub.epa.gov/pfate/E_AChemicals.cfm)	117876	Multiple databases containing chemicals, pesticides, companies, products, etc.	Online
United States National Library of Medicine ChemIDplus Advanced (http://chem.sis.nlm.nih.gov/chemidplus)	117766	Chemical names, synonyms, properties and CAS numbers.	Online

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APPENDIX C: RULES TO ASSIST IN CHEMICAL VERIFICATION PROCESS

1.   Historical names may be interchanged with systematic names.

2.   o-,m-,p-,(ortho, meta, and para) descriptors may be replaced with 1,2-, 1,3-, or 1,4-, respectively.

3.   N-, O-, P-, and S- are locants for substitution on these atoms.

4.   Greek and Latin multiplicative prefixes may be interchanged.

	Greek	*Latin*
1/2	hemi-	semi-
1	mono-, mon-	uni-
2	di-	bi-
3	tri-	tri-, ter-
4	tetra-, tetr-	quadri-, quadr-, quater-
5	penta-, pent-	quinque-, quinqu-
6	hexa-, hex-	sexi-, sex-
7	hepta-, hept-	septi-, sept-
*8	octa-, octo-,	octi-
*9	nona-, non-,	novi-
*10	deca-, dec-,	deci-
*11	undeca-,	undec-
*12	dodeca-,	dodec-

*Generally, Greek prefixes are used; the exceptions are for nine and eleven, where the Latin prefix is used.

$ Bi-, ter-, etc., are employed in ring structures. Bis-, tetrakis-, etc., are used for complex functionality, for example the fusion of rings. They multiply the heading functionality (Biscyclohexa-).

5.   Formal element names may be interchanged with a form of the common name.

Antimony	Sb	Stibium
*Copper	Cu	Cuprum
Gold	Au	Aurum
*Iron	Fe	Ferrum
*Lead	Pb	Plumbum
Mercury	Hg	Hydrargyrum
Silver	Ag	Argentum
Sodium	Na	Natrium
Tungsten	W	Wolframite
*Tin	Sn	Stannum

*Denotes the most common interchanges

6.   Hydrated metal compounds should be assigned CAS numbers of the associated

anhydrous compound (e.g., CuSO4A5H$_2$O should be assigned the CAS number for CuSO4). A comment should be made in the chemical characteristics data field reporting the hydrated form used. Sometimes the author reports a common or trade name for a product that is hydrated, (e.g. Borax, B4Na2O7.10H2O). The paper should be coded to the hydrated CAS number rather than to the anhydrous form as there is no cue for review staff that the compound is hydrated. If the paper were to report it as Sodium borate decahydrate (another name for borax), it would be coded to the anhydrous product as per the text for hydrates mentioned above.

The "ph" in sulfur (sulphur) or sulfur derived names will use an "F" instead of "ph."

7. If a CAS number is verified for a racemic mixture (generic) compound and the isomeric forms are unable to be verified, have the review staff code the isomeric forms under the racemic mixture (generic) CAS Number and note the isomeric form in the Chemical Characteristics data field. Archive the unverifiable isomeric forms and track the references associated with the isomeric form.

8. If a CAS number cannot be verified for a compound (e.g.Silvex ester) but the concentration is based on the active ingredient (AI) or acid equivalent (AE) (e.g. Silvex) OR measured concentrations are presented, code as the AI or AE chemical name (e.g. Silvex). Silvex ester would be archived under the "Archive - Under AI". If neither instance occurs, the chemical will be archived (exception noted in example number 9)

9. If the compound reported results in numerous CAS number options (e.g. MCPA ester) but the concentration is not based on the active ingredient nor are measured concentrations reported, MCPA ester can be coded using the most generic CAS number. For example, MCPA ester results in two possible CAS number options: MCPA 2-ethylhexyl ester – CAS 29450451 and MCPA isooctyl ester – CAS 26544207. In this case, CAS 26544207 would be selected for coding as it is the more generic structure in that the ethyl placement is not defined within the structure.

10. If the paper presents two chemical names for the same compound and one of the names cannot be verified but the other name is verified, code the chemical under the verified name, noting the unverified name in chemical comments (e.g. Paper reports Maneb as Dicotan M22, code as Maneb noting Dicotan M22 in chemical comments).

11[1]. Phrases with "of" included may be rewritten to omit "of." For example, Alkanolamine salt of 2,4-dichlorophenoxy acetic acid as 2,4-Dichlorophenoxy acetic acid alkanolamine salt.

12[1]. Non-English names should be translated into English. This can be done through the use of English-non-English chemical dictionaries at the University of Minnesota-Duluth library, reference section.

13[1]. Names containing letters and numbers should follow these rules:

• The compound name should be first followed by letters and numbers.

>Aliquat 335
>
>Fenthion S2145

- "Compound" and "Substance" should be omitted.

  >B713 not Substance B713

- Company names should be omitted when with letter or number codes.

  >GC 4072 not General Chemical 4072
  >
  >AC 84777 not AC 84777 (American Cyanamid)
  >
  >BAY 5097 not Bayer 5097

- Adjectives describing a compound are not included.

  >Liquor ammonia as Ammonia
  >
  >Organic phosphorus as Phosphorus

14. Pay special attention to papers that report three or four letter chemical names (e.g. DNP). DNP exists under multiple CAS numbers. If the paper only provides an acronym (e.g. DNP) and doesn't provide any additional information such as chemical name/structure, the chemical should be archived.

15. Chemical formulations containing a safener should be verified as a single compound. For example, Puma Super contains Fenoxaprop-p-ethyl. Mefenpyr-diethyl is the safener. It was verified under the CAS number for Fenoxaprop-p-ethyl-mefenpyr-diethyl mixture rather than Fenoxaprop-p-ethyl alone. STN categorizes products containing safeners as mixtures (under a single CAS Number) and they should be notified if a discrepancy is found.

16. Compounds that contain the prefix dextrorotatory (d)- or levorotatory (l)- can also be replaced with (+) – or (-) – respectively. For example: d-2-butanol can also be called (+)-2-butanol and l-2-butanol can also be called (-)-2-butanol. (From p. 346-347 of Wade Jr., L.G, Organic Chemistry)

17. If the paper reports a generic compound but does not specify the form used (e.g. Valproate or Ricinoleate can be salts or esters of Valproic acid and Ricinoleic acid respectively), the paper can be skimmed/coded to the acid form (e.g. Paper reports Valproate which could not be verified. It should be skimmed/coded to Valproic acid with a note placed in the Chemical Characteristics data field regarding the use of Valproate). The unverified chemical should be Archived under AI.

[1]STN International rules paraphrased

APPENDIX D: STN SEARCH INSTRUCTIONS

The following procedure is used to search STN online:

To conduct a search you must obtain a LOGIN ID and PASSWORD from STN International.

1. Open STN and logon by clicking the telephone icon.
2. Capture the session in transcript (filed by month and year). Choose to append to the current month's file if it already exists. If not, open a new file and label it for the current month and year. Click open to start the session
3. Searching by CAS #:
   A. At the prompt, type "fil lreg" (enter). This opens the learning registry.
   B. Type "e (CAS #)/rn" (enter). Example: "e 869-29-4/rn"
   C. In the results, line E3 is what you searched for. The second number is how many results there are for each line.
   D. If results exist for what you expanded, search for that file by typing "s (line #)" (enter). Example: "s e3" searches for the results in line E3.
   E. To display the search results, type "dis" (enter).
   F. The results are displayed. Move immediately on to the next search. The results can be displayed offline later.
4. Searching by chemical name or synonym:
   A. At the prompt, type "fil lreg" (enter).
   B. Type "e (chemical name)/cn" (enter). Example: "e chlorophenol/cn"
   C. Follow steps c-f from above.
5. If searches in the learning registry do not come up with results, search the registry files. This should only be done after first searching the learning registry files. At the prompt, type "fil reg" to open the registry files. All other commands are the same as the learning registry files.
6. To log off STN when all searches are complete:
   A. Type "dis cost" (enter). This displays the total cost of the session. The cost of all sessions should be recorded in a log.
   B. At the prompt, type "log off y" (enter). This logs you off from STN online.
7. After logging off, all results can be displayed offline.

APPENDIX E: SMILES TUTORIAL

What is SMILES?

SMILES (**S**implified **M**olecular **I**nput **L**ine **E**ntry **S**ystem) is a chemical notation that allows a user to represent a chemical structure in a way that can be used by the computer. SMILES is an easily learned and flexible notation. The SMILES notation requires that you learn a handful of rules. You do not need to worry about ambiguous representations because the software will automatically reorder your entry into a unique SMILES string when necessary.

SMILES was developed through funding from the U.S. EPA, National Health and Environmental Research Laboratory (NHEERL), Mid-continent Ecology Division (MED-Duluth), to the Medicinal Chemistry Project at Pomona College, Claremont, CA and the Computer Sciences Corporation, Duluth, MN. Several publications discuss SMILES in more detail, including Anderson et al. 1987, Weininger 1988, Weininger et al. 1989, and Hunter et al., 1987.

SMILES has five basic syntax rules which must be observed. If basic rules of chemistry are not followed in SMILES entry, the system will warn the user and ask that the structure be edited or reentered. For example, if the user places too many bonds on an atom, a SMILES warning will appear that the structure is impossible. The rules are described below and some examples are provided. The rules below allow for the representation of a two-dimensional structure of a chemical. For the ASTER and QSAR systems, a two-dimensional depiction is adequate. Other rules are available for chemicals that are structural isomers, but will not be discussed in this basic tutorial.

Rule One: Atoms and Bonds

SMILES supports all elements in the periodic table. An atom is represented using its respective atomic symbol. Upper case letters refer to non-aromatic atoms; lower case letters refer to aromatic atoms. If the atomic symbol has more than one letter the second letter must be lower case. Bonds are denoted as:

-	Single bond
=	Double bond
#	Triple bond
*	Aromatic bond
.	Disconnected structures

Single bonds are the default and therefore need not be entered. For example, 'CC' would mean that there is a non-aromatic carbon attached to another non-aromatic carbon by a single bond, and the computer would identify

the structure as the chemical ethane. It is also assumed that the bond between two lower case atom symbols is aromatic. A blank terminates the SMILES string.

Rule Two: Simple Chains

By combining atomic symbols and bond symbols simple chain structures can be represented. The structures that are entered using SMILES are hydrogen-suppressed, that is to say that the molecules are represented without hydrogens. The SMILES software understands the number of possible connections that an atom can have. If enough bonds are not identified by the user through SMILES notation, the system will automatically assume that the other connections are satisfied by hydrogen bonds. Some examples:

CC	CH_3CH_3	Ethane
C=C	CH_2CH_2	Ethene
CBr	CH_3Br	Bromomethane
C#N	$C\equiv N$	Hydrocyanic acid
Na.Cl	NaCl	Sodium chloride

The user can explicitly identify the hydrogen bonds, but if one hydrogen bond is identified in the string, the SMILES interpreter will assume that the user has identified **all** hydrogens for that molecule.

HC(H)=C(H)(H)   Ethene

Because SMILES allows entry of all elements in the periodic table, and also utilizes hydrogen suppression, the user should be aware of chemicals with two letters that could be misinterpreted by the computer. For example, 'Sc' could be interpreted as a sulfur atom connected to an aromatic carbon by a single bond, or it could be the symbol for scandium. The SMILES interpreter gives priority to the interpretation of a single bond connecting a sulfur atom and an aromatic carbon. To identify scandium the user should enter [Sc].

Rule Three: Branches

A branch from a chain is specified by placing the SMILES symbol(s) for the branch between a parentheses. The string in parentheses is placed directly after the symbol for the atom to which it is connected. If it is connected by a double or triple bond, the bond symbol immediately follows the left parenthesis. Some examples:

CC(O)C	2-Propanol
CC(=O)C	2-Propanone
CC(CC)C	2-Methylbutane

ECOTOX Chemical Verification and Entry Procedure

CC(C)CC(=O)	2-Methylbutanal
c1c(N(=O)=O)cccc1	Nitrobenzene
CC(C)(C)CC	2,2-Dimethylbutane

Rule Four: Rings

SMILES allows a user to identify ring structures by using numbers to identify the opening and closing ring atom. For example, in C1CCCCC1, the first carbon has a number '1' which connects by a single bond with the last carbon which also has a number '1'. The resulting structure is cyclohexane. Chemicals that have multiple rings may be identified by using different numbers for each ring. If a double, single, or aromatic bond is used for the ring closure, the bond symbol is placed before the ring closure number. Some examples:

C=1CCCCC1	Cyclohexene
C*1*C*C*C*C*C1	
or c1ccccc1	Benzene
C1OC1CC	Ethyloxirane
c1cc2ccccc2cc1	Naphthalene

Rule Five: Charged Atoms

Charges on an atom can be used to override the knowledge regarding a valence that is built into SMILES software. The format for identifying a charged atom consists of the atom followed by brackets which enclose the charge on the atom. The number of charges may be explicitly stated ({-1}) or not ({-}). For example:

CCC(=O)O{-1}	Ionized form of propanoic acid
or CCC(=O)O{-}	
c1ccccn{+1}1CC(=O)O	1-Carboxylmethyl pyridinium

References:

Anderson, E., G.D. Veith, and D. Weininger. 1987. *SMILES: A line notation and computerized interpreter for chemical structures.* Report No. EPA/600/M-87/021. U.S. Environmental Protection Agency, Environmental Research Laboratory-Duluth, Duluth, MN 55804

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APPENDIX F: SMILES DESIGNATORS

If a SMILES string cannot be written, a designator is determined. The designator is used in the Chemical Module. The designators are:

- PLM--Polymer
- LRG--Too large for existing program (> 60 non-hydrogen atoms or > 120 characters)
- GEN--Generic Chemical (e.g. Cresol)
- CMM--Commercial mixture (PhosFlex 400)
- MXT--Generic mixture (Polyoxyethylene gylcols)

APPENDIX G: DELETED/ALTERNATE REGISTRY NUMBERS

If a chemical in Unify is found to be listed under a deleted registered (DR) or alternate registered (AR) CAS number, the following steps should be taken:

1) Enter and verify the Preferred CAS Registry number in Unify, if needed.

2) Check to see if the Deleted or Alternate Registry number exists in the Chemical Module.

   a. If the Deleted or Alternate Registry number exists in the Chemical Module, ensure that there are not any references attached to the record. If no references are attached, select the DR/AR button from the Status Section. If references are attached, data maintenance staff needs to be alerted as they are the ones who would update the references to the Preferred Registry number (this is especially important for reviewed papers. Unreviewed papers could be updated by chemical staff). Once all references are updated, select the DR/AR button from the Status Section.

   b. Once all of the data has been updated in Unify, add the deleted and/or alternate CAS numbers to the Preferred Registry number's Historical CAS tab.

   c. "AR/DR # XXX-XX-X, all records have been updated to Preferred Registry # XXXXXXXXXX" should be added to the Notes tab of the Preferred Registry number.

   d. If the Deleted or Alternate Registry number does NOT exist in the Chemical Module, add the deleted and/or alternate CAS numbers to the Preferred Registry number's Historical CAS tab.

APPENDIX H: VALID CODE CREATION

Staff members that are tasked with creation of codes must have Administration privileges to access "Lookup Codes" in Unify. Please review the general procedures outlined in the ECOTOX Valid Code Creation SOP for a better understanding of the code creation process (N:\ECOTOX SOPs\REVIEW\valid codes\ECOTOX Valid Code Creation.doc).

The following codes are created by Chemical Verification staff during the chemical verification process or reviewing process; Chemical Group, Chemical Property Units, Chemical Use, Chemical TMOA (Toxic Mode of Action), Chemical Formulation, Chemical Grade, Ions, and Radiolabel.

Chemical Group

Code file name: Chemical Group Codes (codes made during Chemical Verification)

Chemical Groups are defined by either a Chemical of Concern (COC) code, a specific project (e.g. EFED) code or by chemical element, e.g. As – Arsenic. Typically, the code created is one that best captures that specific group or COC. For example, if a new COC code is needed, one might use a combination of character s within the chemical name to create a 3 or 4 letter code (e.g. the COC code for Imidacloprid is IMC).

Chemical Property Units

Code file name: Chemical Property Unit Codes (codes made as needed)

Chemical Properties can be found in the Properties tab within the Chemical Module and consist of Molecular Weight, Melting Point, etc. There is no standard practice for creation of these codes. However, ensure sure that abbreviations used for all parts of the unit code are the same as was used for similar units. A search of the already existing codes for these should be done (for example if adding grams/liter it should be verified as g/L rather than as gm/L in order to be consistent with how Grams and Liters are presented in other Unify data fields).

Chemical TMOA (Toxic Mode of Action)

Code file name: Chemical TMOA Codes (static code list, no new codes)

TMOA codes can be found in the Properties tab within the Chemical Module. They are defined as a common set of physiological and behavioral signs that characterize a type of adverse biological response (e.g. non-polar narcosis). Toxic Mode of Action codes are static and only used in the ASTER application. If/when new TMOAs are developed/approved by EPA, new TMOAs will be added to Unify.

Chemical Use

Code file name: Chemical Use Codes (static code list, no new codes)

It defines the common use(s) for a pesticide active ingredient (e.g. herbicide). The use is added if it can be determined from verification sources. The most common is PAN (http://www.pesticideinfo.org/Search_Chemicals.j_sp). STN will also sometimes provide this information. Currently the Chemical Use is a static code list. If/when additional Chemical Uses are located, they will require programmer's assistance in updating the "target Logic" that is contained in Unify to prioritize coding for special projects; typically the code created is one that best captures the chemical use description (e.g. FUMI is the code for Fumigant).

Chemical Formulation

Code file name: Chemical Formulation Codes (codes made as needed during review process)

Chemical Formulation is the way in which the chemical is prepared. These codes are created with two or three characters that best captures the formulation description (e.g. AI is Active Ingredient).

Chemical Grade

Code file name: Chemical Grade Codes (codes made as needed during review process)

Chemical Grade reflects the quality of the product. Different industries have different standards for chemical grades depending upon the purpose (for example ACS Grade is a "grade of highest purity and meets or exceeds purity standards set by American Chemical Society (ACS)" - http://www.sciencecompany.com/Learn-Chemical-Grade-Definitions-from-Highest-to-Lowest-Purity-W53.aspx/.

These codes are created with two or three characters that best captures the grade description (e.g. ACS is American Chemical Society Grade).

Ions

Code file name: Ion Codes (codes made as needed during review process)

This code is used when the chemical concentration is based upon an ionic form of a chemical . Typically these codes are used for Metal compounds and are comprised of elemental symbols (e.g. Cd for Cadmium). However, there are occasions where ions may be needed for Organic compounds such as Paraquat or other chemicals that tend to dissociate such as Ammonium. These codes are created using a few characte rs that best capture the ion description.

Radiolabel

Code file name: Radio Label Codes (codes made as needed during review process)

This code is used if radiolabeled products are tested . The standard code convention for a nucleus (e.g. ^{12}C) is to use the elemental symbol followed by a dash and then the atomic mass unit. For example, ^{12}C has the code of C-12.